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Project Summary

Rocky Mountain Acid Deposition Model Assessment: Review of Existing Mesoscale Models for Use in Complex Terrain

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Existing mesoscale meteorological and acid deposition models are surveyed, reviewed, and evaluated for potential application to a complex terrain region within the Rocky Mountain region. The purpose of the review it to choose meteorological and acid deposition models that might be inclued in a mesoscale acid deposition model for the Rocky Mountain region. This acid deposition model would then be used by the western regulatory agencies to estimate the amounts of acidic deposition from proposed new sources at PSD class 1 and acid-sensitive areas.

Typical application scenarios consist of shale oil plants and gas treatment plants that emit both sulfur and nitrogen oxides. Thus it will be important to correctly define the source-receptor relationship of both sulfur and nitrogen deposition over mesoscale distances in complex terrain. The project report includes a review of meteorological modeling in complex terrain and acid deposition processes, a survey of over 60 existing mesoscale meteorological and acid deposition models, and a discussion of the procedures used to select candidate meteorological and acid deposition models for final evaluation. Among the candidate models, no one meteorological or acid deposition model was significantly superior to the others; all the candidate models contained different features that would be desirable attributes in an acid deposition model for the Rocky Mountain region. The conceptual design of the mesoscale acid deposition model makes use of modules from the candidate meteorological and acid deposition models.

This Project Summary was developed by EPA's Atmospheric Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Acid deposition has recently become an increasing concern in the western United States. Although this problem may not be as acute in the western United States as it is in the eastern United States, it is currently a concern of the public and regulatory agencies because of the high sensitivity of western lakes at high altitudes and the rapid industrial growth expected to occur in certain areas of the West. An example of such an area is the region known as the Overthrust Belt in southwestern Wyoming. Several planned energy-related projects including natural gas sweetening plants and coal-fired power plants may considerably increase emissions of acid precursors in northeastern Utah and northwestern Colorado and significantly affect ecosystems in the sensitive Rocky Mountain areas.



Under the 1977 Clean Air Act, the U.S. **Environmental Protection Agency** (EPA), along with other federal and state agencies, is mandated to preserve and protect air quality throughout the country. As part of the Prevention of Significant Deterioration (PSD) permitting processes, federal and state agencies are required to evaluate potential impacts of new emission sources. In particular, Section 165 of the Clean Air Act stipulates that, except in specially regulated instances, PSD increments shall not be exceeded and air quality-related values (AQRV's) shall not be adversely affected. Air-quality-related concerns range from near-source plume blight to regional-scale acid deposition problems. By law, the Federal Land Manager of Class I areas has a responsibility to protect air-quality-related values within those areas. New source permits cannot be issued by the EPA or the states when the Federal Manager concludes that adverse impacts on air quality or airquality-related values will occur. EPA Region VIII contains some 40 Class I areas in the West, including two Indian reservations. Several of the remaining 26 Indian reservations in the region are considering similar designations. State and federal agencies, industries, and environmental groups in the West need accurate data concerning western source-receptor relationships.

To address this problem, EPA Region VIII needs to design an air quality model for application to mesoscale pollutant transport and deposition over the complex terrain of the Rocky Mountain region for transport distances ranging from several km to several hundred km. The EPA recognizes the uncertainties and limitations of currently available air quality models and the need for continued research and development of air quality models applicable over regions of complex terrain. Therefore, the objective of the project reported here is to select and assemble the best air quality models available for application to the Rocky Mountain area.

Air quality modeling of the Rocky Mountain region is especially difficult due to the complex airflow patterns over the Rocky Mountains and the difficulty of predicting acid deposition levels. Available data bases are inadequate for thorough model evaluation studies.

The primary objective of this project is to assemble an interim air quality model based primarily on models or modules currently available for use by the federal and state agencies in the

Rocky Mountain region. The EPA has formed an atmospheric processes subgroup of the Western Atmospheric Deposition Task Force, referred to as WADTF/AP, to develop criteria for model selection and subsequent model evaluations. This group comprises representatives from the National Park Service, U.S. Forest Service, EPA, Region VIII, the National Oceanic and Atmospheric Administration, and other federal, state, and private organizations. On the basis of our review of the modeling needs identified by the WADTF/AP, the specific requirements of the model proposed in this project are as follows:

The anticipated use of the model is to analyze permit applications by calculating acid deposition impacts at sensitive receptors from specified sources. Thus the primary need is to estimate long-term averages of wet and dry nitrogen and sulfur deposition amounts. However, there is also a need to estimate short-term (3-hour, 24-hour) SO₂ and TSP impacts for PSD increment consumption. Thus the model should be primarily concerned with a mesoscale region within the Rocky Mountain region.

The modeling system will include a mesoscale meteorological model, which creates wind fields in complex terrain, as a driver for an acid deposition model. Since the primary interest is in longer-term averages, this meteorological model will be required to generate these wind fields in a cost effective manner.

The acid deposition model will be primarily concerned with estimating incremental acid deposition and ambient concentration impacts from the specified sources only.

A mathematical modeling system for describing the various physical and chemical processes associated with acid deposition must consist of several components or modules. These modules describe processes such as wind transport, chemical reactions, plume rise, and wet/dry deposition. Although the modeling system must be an integrated, internally consistent package, it can be conveniently divided into two distinct parts:

Simulation of meteorological processes

Simulation of pollutant dispersion, chemical reactions, and deposition.

Procedure

After an extensive literature review, 65 mesoscale meteorological and 75

acid deposition/air quality models were identified as possible candidates for incorporation into an acid deposition model for the Rocky Mountain region. These models were classified according to their model formulation, and parameterizations of the major processes that describe airflows or acid deposition over complex terrain. Those meteorological models that did not treat complex terrain were eliminated from further consideration. The remaining models were then subjected to a technical merit analysis in which objective scores are assigned to the modeling approaches to the processes that lead to airflows over complex terrain and acid deposition. A model ranking was obtained by summing the scores the model receives for the treatment of the major processes.

The needs and desires of the potential users were considered in the selection process. The most technically advanced model may not be the most appropriate choice if it does not meet the needs of the users. Based on such nontechnical criteria, the final candidate meteorological and acid deposition models were chosen for further analysis.

The mesoscale meteorological models were subjected to a comparative evaluation and then exercised using a hypothetical terrain obstacle at a scale typically found in the Rocky Mountair region. The acid deposition models were evaluated by a detailed analysis of the methods used by the models to treatransport, diffusion, chemical transformation, and dry and wet deposition.

Results and Discussion

Review of Mesoscale Meteorological Models

The alteration of large-scale wind flows by terrain features can be roughly divided into kinematic, dynamic, and thermal-radiational effects. The kine matic effects are a result of the deflect tion of the synoptic wind due by the ter rain. Kinematic effects include blocking channeling, and orographic lifting. Dy namic effects are caused by the interact tion of the mountain topography an the atmosphere. Under stable cond tions, air forced vertically over a ridg may oscillate in an internal gravity way called lee waves. Another dynamic e fect involves the degree of coupling be tween synopytic winds, and the winc within valleys and canyons. Thermal e fects are caused by the heating or coc ing of the ground surface, which cause

air parcels near the ground to rise or fall. Examples of thermal effects include katabatic, or drainage winds, that are driven by the gravity force as the higher terrain becomes an elevated heat sink due to long-wave radiation, the colder air moves downslope. Similarly, upslope or anabatic winds during the day are driven by buoyancy forces as the higher terrain becomes an elevated heat source in response to solar heating. In reality, airflows in complex terrain are a result of a combination of the synoptic wind and the kinematic, dynamic, and thermal effects. The degree to which a mesoscale meteorological model can simulate these phenoma is an important factor in the selection of the model.

We identified 65 models that have the potential of describing meteorological processes in the atmosphere. These meteorological models consisted of 50 prognostic models based on the primitive equations or the vorticity formulation, 12 diagnostic models based primarily on the conservation of mass equation, and three objective analysis interpolation schemes. The prognostic models are technically more rigorous because they explicitly solve the coupled differential equations of conservation of mass, heat, water, and momentum. Although less technically sound than the prognostic models, the diagnostics models have been used more extensively in the past for air pollution studies because they are able to produce mass-consistent wind fields that match observations in a cost-effective manner. The objective analysis interpolation procedure has also been used frequently in air pollution models in the past; however, the procedure requires extensive measurements to properly describe airflows, and may not be appropriate for applications to complex terrain where observations are limited.

The candidate mesoscale meteorological models are first classified according to their mathematical formulation and the parameterizations of the major processes. Since the primary purpose of the meteorological models will be to generate wind fields over complex terrain to drive an acid deposition model, we identified three minimum reguirements for the meteorological model for this project: (1) the model must be able to predict a threedimensional wind field, (2) it must be able to accommodate complex terrain, and (3) it must be currently operational. Of the 65 mesoscale meteorological models surveyed, 17 do not predict a three-dimensional wind field. These models are either one-dimensional, slab-symmetric (x,z), single-layer models (x,y), or models with a Lagrangian formulation. Of the remaining 48 models, 11 do not explicitly account for complex terrain. These models include urban meteorological models, and models used for hurricanes or tropical storms in which terrain can be adequately treated through increased frictional effects. Of the remaining 37 models, 15 were classified as being currently operational. A model was classified as being non-operational if it was developed outside of the United States and the model code or simulation results were deemed too difficult to obtain, or if it was reported as a research-grade model in the literature.

The remaining 15 models consisted of six prognostic models based on the primitive equations, one diagnostic model based on the primitive equations, and eight diagnostic models based on mass continuity. Candidate mesoscale meteorological models were selected on the technical merits of the models and the needs of the potential users. The need for generating wind fields on a long-term temporal scale precludes the use of the prognostic models, and the diagnostic model based on the primitive equations. The choice of the final candidate meteorological models was based on a technical merit analysis in which scores were assigned to the models' mathematical formulation, data reliance, and treatment of the phenomena of blocking, kinematic effects, mountain waves, and upslope/downslope effects.

The evaluation of the four final candidate mesoscale meteorological models consisted of a comparative description of the models' treatment of the initialization procedure and adjustment to mass conservation, and by simulations using a hypothetical terrain obstacle at a scale found in the Rocky Mountains. The results of the evaluation of the candidate meteorological models indicated that no one model was superior to the others. If there is a total lack of observational data, the SAI/CTWM alone among the candidate models is able to generate wind fields. However, the SAI/ CTWM is also the only model formulated in a Cartesian coordinate system, an undesirable attribute, and the ability of the model to use more than one wind observation is questionable. For the treatment of blocking and deflection of air flows, both the PNL/MELSAR-MET and the SAI/CTWM contain Froude Froude number adjustments. If reasonable vertical velocities are desired, then the LANL/ATMOS1, which attempts adjustment of the vertical velocity based on stability criteria, may be a better choice. If input data is plentiful and representative, the flexibility of the CIT/WINDMOD interpolation scheme may be of value.

The design of the meteorological model as a driver for an acid deposition model for the Rocky Mountain region requires the generation of other meteorological variables, in addition to wind fields. Of the final candidate meteorological models, only the PNL/MELSAR-MET also generates gridded fields of boundary layer heights, temperatures, and other meteorological variables. Thus the conceptual design makes use of the PNL/MELSAR-MET code as a basis for the meteorological driver. However, the wind field module within the PNL/MELSAR-MET may be replaced by another candidate model formulated in a terrain-following coordinate system. Whichever model is chosen, some of the unique upslope/downslope parameterizations within the SAI/ CTWM will be added.

Review of Existing Acid Deposition/Air Quality Models

Acid deposition/air quality models can be divided into long-term and episodic models. Long-term models generally are either deterministic models, which calculate the average of individual simulations of all episodes for the time period of interest, or statistical models, which calculate a long-term average based on the mean of individual trajectory calculations or long-term average (climatological) data. Episodic models can be classified according to the fixed-frame Eulerian models, the moving-framework Lagrangian models, or hybrid models that merge aspects of both Eulerian and Lagrangian models. Lagrangian models can be further divided into forward trajectory (source oriented), or backward trajectory (receptor oriented) models. For the purpose of simulating source-receptor relationships over mesoscale distances in complex terrain, the use of statistical models may not be appropriate. Since nonlinear chemical transformation cannot be simulated with the Lagrangian backward trajectory approach, the most appropriate modeling methodology appears to be the deterministic approach

within either an Eulerian or sourceoriented Lagrangian modeling framework.

The physical and chemical processes that determine the fate of natural and anthropogenic acid precursors are numerous, complex, and intertwined. Successful modeling of pollutant deposition requires simulating the most important of the processes and interactions. For the purpose of constructing an acid deposition model for the Rocky Mountain region, the most important processes can be divided into transport, dispersion, chemical transformation, and dry and wet deposition.

Over 75 acid deposition/air quality models were surveyed and reviewed as to their input/output data requirements, transport and dispersion algorithms, formulation of chemical transformation, and treatment of wet and dry deposition. In order to rank the models, a technical merit analysis assigned scores to the methods used to treat the major processes that lead to acid deposition. Based on technical merit alone, the 10 highest-ranking acid deposition/air quality models were retained for further consideration.

The requirements of the potential users are that only source-specific impacts be calculated and that these estimates must be made in a cost-effective manner. Although Eulerian models may be technically superior in simulating cumulative acid deposition, they are not as cost-effective as Lagrangian models for calculating source-specific impacts. Thus, based on the needs of the potential users, the candidate acid deposition models for the Rocky Mountain region are the four highest ranking Lagrangian models: ERT/MESOPUFF-II, PNL/MELSAR-POLUT, SAI/CCADM, and SAI/RIVAD.

The four candidate models were evaluated for their treatment of transport, dispersion, chemical transformation, and dry and wet deposition. None of the models contained a superior treatment in all of these categories. Thus the conceptual design of the acid deposition model for the Rocky Mountin region will make use of components from each of these models. The conceptual design makes use of the Gaussian puff formulation as used in the POLUT and MESOPUFF-II. Transport of the puff would be defined by the meteorological model. The dispersion coefficients within the POLUT model will be used for diffusion since they contain the best representation of dispersion over complex terrain. Chemical transformation will be obtained from a parameterized version of the chemistry module in CCADM. This model contains one of the most up to date gas-phase and aqueous-phase chemical kinetic mechanisms. Dry deposition would be based on modules in the MESOPUFF-II or the CCADM. The dry deposition algorithms in these models use the preferred resistance approach. The selection of the final module will depend on tests using data characteristics from the Rocky Mountain region. Wet deposition will be based on the scavenging coefficient concept. This approach is more consistent with the Lagrangian model formulation and the varying effects of scavenging due to rain, snow, and storm type can be easily incorporated.

Conclusions and Recommendations

The acid deposition model for the Rocky Mountain region developed in this project will have the following attributes: (1) the model is designed for use by Western regulatory agencies to estimate source-specific acid deposition

impacts at acid-sensitive receptors; (2) the model is based on existing models and modules; (3) the model uses a Lagrangian model formulation; and (4) the model is designed specifically for complex terrain.

The model is intended to be used as an aid in deciding PSD permits. The model should undergo testing and evaluation in order to establish confidence in the results. The meteorological model should be tested against field data and the performance of other models using a wide variety of meteorological conditions. The acid deposition should be evaluated against field tracer data in flat and complex terrain, both with and without the meteorologica driver. During simplified conditions (flat terrain, inert tracer) the model should produce results that are similar to those generated by existing regulatory mod els. Finally, the model should be sub jected to an extensive sensitivity analy sis in order to understand the relative importance of the definition of the inpu parameters. The authors recognize the limitations of these types of models.

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The complete report entitled "Rocky Mountain Acid Deposition Model Assessment: Review of Existing Mesoscale Models for Use in Complex Terrain," (Order No. PB 87-180 584/AS; Cost: \$36.95, subject to change) will be available only from.

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